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S=O...S=O Interactions as a Driving Force for Low-Temperature Conformational Rearrangement of Stable H-Bonding {S(O)-Ch2-Ch2-OH···}2 Synthon in two Modifications of Diastereomeric Pinanyl Sulfoxides Co-Crystal

Lodochnikova O., Krivolapov D., Startseva V., Nikitina L., Bodrov A., Artemova N., Klochkov V., Madzhidov T., Chmutova G., Litvinov I.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Copyright © Taylor & Francis Group, LLC. (Graphical Abstract) For the triclinic and monoclinic modifications of diastereomeric pinanyl sulfoxides co-crystal, remarkable alterations in unit cell parameters by transition from 293 to 150 were ascertained. Such alterations are accompanied by conformational restructuring of a stable hydrogen-bonded synthon from an "unfolded" to a "folded" form. The driving force of this restructuring is the tendency to form S=O.S=O interactions, which show up in the lowerature phases of both polymorphs. These are well-supported by the methods of quantum chemistry (DFT, B97-D/6-31G(d,p), AIM All).

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Keywords

"racemic compound-like" crystallization, -β-pinene, hydrogen-bonded cyclic dimers, lowerature X-ray structural analysis, polymorphic modifications, β-Hydroxy sulfoxide